A Fourier–Bessel Expansion for Solving Radial Schrödinger Equation in Two Dimensions

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ABSTRACT

The spectrum of the two-dimensional Schrödinger equation for polynomial oscillators bounded by infinitely high potentials, where the eigenvalue problem is defined on a finite interval $r \in [0, L)$, is variationally studied. The wave function is expanded into a Fourier–Bessel series, and matrix elements in terms of integrals involving Bessel functions are evaluated analytically. Numerical results presented accurate to 30 digits show that, by the time L approaches a critical value, the low-lying state energies behave almost as if the potentials were unbounded. The method is applicable to multiwell oscillators as well.

1. Introduction

In his recent articles [1–3], Taşeli modified the usual requirement that the wave function should tend to zero at infinity and showed that the eigensolution of the Dirichlet boundary value problem can be effectively used to find the spectrum of an unbounded problem in one dimension. In these works, the eigenfunctions satisfying the boundary value problem

$$\frac{d^2\Psi}{dx^2} + \mu^2\Psi = 0, \qquad \Psi(a) = \Psi(b) = 0 \quad (1.1)$$

were employed as the basis set in the Rayleigh–Ritz variational method. The approach has a natural extension to the two-dimensional Schrödinger equation written in Cartesian coordinates. Actually, two-dimensional anharmonic oscillators can be treated in a similar fashion by means of the boundary value problem defined by

$$\frac{d^2\Psi}{dx^2} + \frac{d^2\Psi}{dy^2} + \mu^2\Psi = 0, \qquad \Psi|_\Gamma = 0, \quad (1.2)$$

where Γ denotes the boundary of a finite rectangular region in the xy-plane [4].

In this study, we examined the dimensionless radial Schrödinger equation in the cylindrical polar

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coordinates:

$$\left[-\frac{d^2}{dr^2}-\frac{1}{r}\frac{d}{dr}+\frac{l^2}{r^2}+V(r)\right]\Psi(r)=E\Psi(r),$$

$$r\in[0,\infty), \quad (1.3)$$

where $l=0,1,\ldots,V(r)$ and E stand for the magnetic quantum number, the potential function, and the energy eigenvalue, respectively. It is obvious that the coupling might depend on the direction. We have, however, omitted the angle dependence of the potential for the sake of dealing with a system which can be investigated via an ordinary differential equation. Therefore, l characterizes the angular dependence of the system in a global sense, and the wave function Ψ has been regarded as a function of the single variable r.

The accompanying boundary conditions of (1.3) are the regularity and the appropriately vanishing behavior of the wave function specified as $r\to 0$ and $r\to\infty$, respectively. The regularity condition implies that

$$\Psi(r)=O(r^l) \quad (1.4)$$

as $r\to 0$. The second condition, however, is replaced by

$$\Psi(L)=0 \quad (1.5)$$

when the interval is truncated to $[0, L]$. Such a truncation is clearly motivated by the success of the simple technique presented in the aforementioned articles [1–4]. The question which now arises is whether there exists a corresponding basis set, preferably in terms of elementary or special functions of mathematical analysis for solving (1.3). Fortunately, in the case of the radial Schrödinger equation, the Bessel functions of the first kind are to be shown in Section 2 to play the same role with the trigonometric basis.

The potential function $V(r)$ in (1.3) is taken as a general polynomial:

$$V(r)=\sum_{j=1}^{M} v_{2j}r^{2j}, \qquad v_{2M}>0, \qquad M=1,2,\ldots \quad (1.6)$$

in r^2. The positiveness of the dominant coupling constant v_{2M} is sufficient to make the potential bounded below. Therefore, the operator being considered has now a purely discrete spectrum. The special case of the harmonic oscillator, $V(r)=r^2$, admits exact solutions in the unbounded domain of r of the form

$$\Phi_{nl}(r)=e^{-(1/2)r^2}L_n^{(l)}(r^2), \qquad E_{n,l}=2(2n+l+1), \quad n,l=0,1,\ldots, \quad (1.7)$$

where $L_n^{(l)}$ denotes the associated Laguerre polynomials.

In general, the asymptotic behavior of the wave function as $r\to\infty$ completely depends on the dominant coupling. As a result, it is rather difficult to introduce a trial function reflecting the desired properties of the solution for an arbitrary anharmonic interaction [5]. The definition of the problem in a finite interval $r\in[0, L]$, however, makes it possible to consider a general polynomial potential rather than a specific one. The idea is based upon regarding the boundary value L as a nonlinear optimization parameter to be determined in such a way that the spectrum fits to the spectrum of the corresponding unbounded problem, where $L\to\infty$, to any prescribed accuracy. Moreover, a model of this kind, namely, an enclosed quantum mechanical system, is of importance not only for finding the spectrum of an unbounded one but also its various applications in several fields [6] (and the references cited therein).

Within these perspectives, Section 2 sets out the basic variational formulation of the problem. Section 3 includes the evaluation of integrals containing Bessel functions. The last section presents the applications of the method and concludes the article with a discussion of the results.

2. The Fourier–Bessel Expansion

In this section, we begin with solving the unperturbed Schrödinger equation defined by

$$\left(\frac{d^2}{dr^2}+\frac{1}{r}\frac{d}{dr}+\mu^2-\frac{l^2}{r^2}\right)\Phi(r)=0, \qquad r\in[0,L], \quad (2.1)$$

subject to

$$\Phi(r)=O(r^l) \quad \text{as } r\to 0, \qquad \Phi(L)=0, \quad (2.2)$$

where μ is a constant, and we have assumed a potential function of the form

$$V(r)=\begin{cases}0, & 0\le r<L\\ \infty, & r>L.\end{cases} \quad (2.3)$$

It is readily shown that the two linearly independent solutions of (2.1) are $J_l(\mu r)$ and $Y_l(\mu r)$, namely, the Bessel functions of the first and the second kind, respectively. However, the Bessel functions of the second kind do not remain finite at $r = 0$ so that we may take

$$\Phi(r) = cJ_l(\mu r), \tag{2.4}$$

which behaves correctly at the origin, where c is some normalization constant. More specifically,

$$\Phi(r) \approx \frac{c\mu^l}{2^l l!} r^l \tag{2.5}$$

as $r \to 0$. Imposing the second condition, we see that (2.4) is the required solution if μ is a positive root of the equation

$$J_l(\mu L) = 0. \tag{2.6}$$

We know from the theory of Bessel functions that there is an enumerable infinite set of roots $\mu = \mu_1, \mu_2, \ldots \mu_n, \ldots$ satisfying (2.6) [7]. Furthermore, when c is properly chosen, the sequence of functions

$$\Phi_n(r) = \frac{\sqrt{2}}{LJ_{l+1}(\mu_n L)} J_l(\mu_n r), \qquad n = 1, 2, \ldots \tag{2.7}$$

forms an orthonormal set over the range of r, $r \in [0, L]$, with respect to the weighting function r. Thus, we have

$$\int_0^L r\Phi_n(r)\Phi_m(r)\, dr = \delta_{nm} \tag{2.8}$$

for all values of n and m.

The orthonormality property suggests the expansion of the wave function in the form

$$\Psi(r) = \sum_{n=1}^{\infty} a_n \Phi_n(r) = \frac{\sqrt{2}}{L} \sum_{n=1}^{\infty} \frac{a_n}{J_{l+1}(\mu_n L)} J_l(\mu_n r), \tag{2.9}$$

which is called the Fourier–Bessel expansion of $\Psi(r)$. The theory of such an expansion is given by Watson in [8]. Substituting (2.9) into (1.3), multiplying the result by $r\Phi_m(r)$, and integrating from zero to L, we obtain

$$\sum_{n=1}^{\infty} \left[\mu_n^2 \delta_{nm} + \int_0^L V(r) r \Phi_n(r) \Phi_m(r)\, dr - E\delta_{nm} \right] a_n = 0, \tag{2.10}$$

for $m = 1, 2, \ldots$. If we define the variational matrix to be

$$H_{nm} = \mu_n^2 \delta_{nm} + \int_0^L V(r) r \Phi_n(r) \Phi_m(r)\, dr, \tag{2.11}$$

we then arrive at the secular equations of the form

$$\sum_{n=1}^{\infty} (H_{nm} - E\delta_{nm}) a_n = 0, \qquad m = 1, 2, \ldots, \tag{2.12}$$

for determination of the coefficients a_n. Using (1.6) and making a simple change of variable, the variational matrix is expressible as

$$H_{nm} = (\alpha_n / L)^2 \delta_{nm} + \sum_{j=1}^{M} v_{2j} L^{2j} I_{nm}^{(l,j)}, \tag{2.13}$$

wherein $I_{nm}^{(l,j)}$ stands for the integral

$$I_{nm}^{(l,j)} = c_{nm}^{(l)} \int_0^1 \xi^{2j+1} J_l(\alpha_n \xi) J_l(\alpha_m \xi)\, d\xi \tag{2.14}$$

to be determined for each l. Hereafter, $\alpha_1, \alpha_2, \ldots, \alpha_n, \ldots$ denote the positive zeros of $J_l(x)$, and the constant $c_{nm}^{(l)}$ is given by

$$c_{nm}^{(l)} = \frac{2}{J_{l+1}(\alpha_n) J_{l+1}(\alpha_m)}. \tag{2.15}$$

It is apparent that $I_{nm}^{(l,j)}$ is symmetric in n and m and, hence, that H_{nm} is symmetric.

In the coming section, we shall show that the integrals in (2.14) may be evaluated recursively. In particular,

$$I_{nm}^{(l,0)} = \delta_{nm} \tag{2.16}$$

provided that $J_l(\alpha_n) = 0$ for any l fixed.

3. Evaluation of Matrix Elements

In this section, the integrals appearing in the matrix elements are evaluated analytically for $l = 0$

and $l = 1$, which are representative for the other cases. Since such integrals are not so trivial to deal with, we feel that we should give a sketch of the derivation steps. So let us consider (2.14) setting $l = 0$,

$$I_{nm}^{(0,j)} = c_{nm}^{(0)} \int_0^1 \xi^{2j+1} J_0(\alpha_n \xi) J_0(\alpha_m \xi)\, d\xi; \qquad n, m = 1, 2, \ldots, \quad (3.1)$$

with $J_0(\alpha_n) = 0$ and $j = 1, 2, \ldots, M$. Integrating by parts and using some well-known properties of the Bessel functions, we see that (3.1) may be written as

$$I_{nm}^{(0,j)} = \frac{2j}{\alpha_n^2 - \alpha_m^2}(\alpha_m A_{mn} - \alpha_n A_{nm}), \quad (3.2)$$

when $n \neq m$, where

$$A_{pq} = c_{pq}^{(0)} \int_0^1 \xi^{2j} J_1(\alpha_p \xi) J_0(\alpha_q \xi)\, d\xi \quad (3.3)$$

and $A_{pq} \neq A_{qp}$. Integration by parts of the last integral leads to

$$\alpha_m A_{nm} + \alpha_n A_{mn} = 2 - 2(j-1) P_{nm}^{(1,j-1)}, \qquad j > 0, \quad (3.4)$$

where a temporary quantity $P_{nm}^{(1,j)}$,

$$P_{nm}^{(1,j)} = c_{nm}^{(0)} \int_0^1 \xi^{2j+1} J_1(\alpha_n \xi) J_1(\alpha_m \xi)\, d\xi, \qquad P_{nm}^{(1,j)} = P_{mn}^{(1,j)}, \quad (3.5)$$

has been introduced. It should be noticed that $P_{nm}^{(1,j)}$ is not a constant multiple of $I_{nm}^{(1,j)}$ defined by (2.14) since α_n's are not the zeros of $J_1(x)$ in this case of $l = 0$. If we now make use of the identity

$$\begin{aligned} \frac{d}{d\xi}\left[\xi^{2j} J_0(\alpha_n \xi) J_0(\alpha_m \xi)\right] &= 2j\xi^{2j-1} J_0(\alpha_n \xi) J_0(\alpha_m \xi) \\ &\quad - \alpha_n \xi^{2j} J_1(\alpha_n \xi) J_0(\alpha_m \xi) \\ &\quad - \alpha_m \xi^{2j} J_0(\alpha_n \xi) J_1(\alpha_m \xi); \end{aligned} \quad (3.6)$$

it follows immediately that

$$\alpha_n A_{nm} + \alpha_m A_{mn} = 2j I_{nm}^{(0,j-1)}, \qquad j > 0, \quad (3.7)$$

which is independent of (3.4). Solving simultaneously (3.4) and (3.7) for A_{nm} and A_{mn} and substituting into (3.2), we find that

$$I_{nm}^{(0,j)} = \frac{4j}{(\alpha_n^2 - \alpha_m^2)^2}\left\{2\alpha_n \alpha_m\left[1 - (j-1) P_{nm}^{(1,j-1)}\right] - j(\alpha_n^2 + \alpha_m^2) I_{nm}^{(0,j-1)}\right\} \quad (3.8)$$

for $j > 0$ and $m \neq n$. Likewise, we obtain the relation

$$\begin{aligned} P_{nm}^{(1,j)} = \frac{4j}{(\alpha_n^2 - \alpha_m^2)^2} &\times \left\{(\alpha_n^2 + \alpha_m^2)\left[1 - (j-1) P_{nm}^{(1,j-1)}\right]\right. \\ &\left. - 2j\alpha_n \alpha_m I_{nm}^{(0,j-1)}\right\} \end{aligned} \quad (3.9)$$

for the calculation of $P_{nm}^{(1,j)}$ recursively. The initial conditions for these recursions are

$$I_{nm}^{(0,0)} = 0 \quad (3.10)$$

and

$$P_{nm}^{(1,0)} = 0, \quad (3.11)$$

respectively. The first condition is a consequence of the orthogonality of the Bessel functions, and the second one can be deduced from the integral (3.5) with $j = 0$.

Whenever $m = n$, $I_{nn}^{(0,j)}$ may be derived by means of certain limit operations as $\alpha_n \to \alpha_m$ using l'Hospital rule. It is, however, easier to follow an alternative way. Indeed, noting that (3.4) and (3.7) are valid for $m = n$ as well, we show that

$$(j+1) I_{nn}^{(0,j)} = 1 - j P_{nn}^{(1,j)} \quad (3.12)$$

and that

$$\alpha_n A_{nn} = j I_{nn}^{(0,j-1)}. \quad (3.13)$$

On integrating by parts, it is not difficult to prove that $P_{nn}^{(1,j)}$ satisfies also the equation

$$\alpha_n (j+1) P_{nn}^{(1,j)} = \alpha_n - j\alpha_n I_{nn}^{(0,j)} + 2jA_{nn}. \quad (3.14)$$

Therefore, substituting (3.13) into (3.14) and eliminating $P_{nn}^{(1,j)}$ from (3.12) and (3.14), it follows that

$$\alpha_n^2 (2j+1) I_{nn}^{(0,j)} = \alpha_n^2 - 2j^3 I_{nn}^{(0,j-1)}, \qquad j = 1, 2, \ldots, M. \quad (3.15)$$

Initially, we have from (2.16)

$$I_{nn}^{(0,0)} = 1 \quad (3.16)$$

for all n.

In a similar fashion, for $l = 1$, the integral

$$I_{nm}^{(1,j)} = c_{nm}^{(1)} \int_0^1 \xi^{2j+1} J_1(\beta_n \xi) J_1(\beta_m \xi)\, d\xi; \qquad n, m = 1, 2, \ldots \quad (3.17)$$

may be evaluated recursively, where the β_n's are now the positive zeros of $J_1(x)$. If $m \neq n$, we find that

$$I_{nm}^{(1,j)} = \frac{4j}{(\beta_n^2 - \beta_m^2)^2}\left\{2\beta_n \beta_m\left[1 - jQ_{nm}^{(0,j-1)}\right] - (j-1)(\beta_n^2 + \beta_m^2) I_{nm}^{(1,j-1)}\right\}, \qquad I_{nm}^{(1,0)} = 0 \quad (3.18)$$

and

$$Q_{nm}^{(0,j)} = \frac{4j}{(\beta_n^2 - \beta_m^2)^2}\left\{(\beta_n^2 + \beta_m^2)\left[1 - jQ_{nm}^{(0,j-1)}\right] - 2(j-1)\beta_n \beta_m I_{nm}^{(1,j-1)}\right\}, \qquad Q_{nm}^{(0,0)} = 0, \quad (3.19)$$

where

$$Q_{nm}^{(0,j)} = c_{nm}^{(1)} \int_0^1 \xi^{2j+1} J_0(\beta_n \xi) J_0(\beta_m \xi)\, d\xi, \qquad Q_{nm}^{(0,j)} = Q_{mn}^{(0,j)}. \quad (3.20)$$

If $m = n$, then

$$(2j+1)\beta_n^2 I_{nn}^{(1,j)} = \beta_n^2 - 2j(j^2 - 1) I_{nn}^{(1,j-1)}, \qquad I_{nn}^{(1,0)} = 1. \quad (3.21)$$

In general, the problem of calculating integrals in (2.14) for any l requires a treatment of this kind.

4. Applications and Concluding Remarks

The present technique is applied to some specific potentials in (1.6) to show its computational performance. To this end, the infinite system (2.14) has been truncated to a homogeneous system of a finite number of equations, N say. The truncated eigenvalues are then determined as the roots of the so-called characteristic equation.

We examine numerically the generalized anharmonic oscillators

$$V(r) = r^2 + v_{2k} r^{2k}, \qquad k = 2, 3, 4, \quad (4.1)$$

and the double-well potential of the form

$$V(r) = -r^2 + d_4 r^4 \quad (4.2)$$

for a wide range of the coupling constants. As $v_{2k} \to \infty$ in (4.1), we have the infinite-field limit Hamiltonian described by the equation

$$\left(-\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} + \frac{l^2}{r^2} + r^{2k}\right)\Psi(r) = \lambda\Psi(r), \quad (4.3)$$

where λ is connected with the energy eigenvalues by the relation

$$\lambda = v_{2k}^{-1/(k+1)} E. \quad (4.4)$$

This asymptotic relation shows that the total energy E of the system (1.3) grows like $v_{2k}^{1/(k+1)}$ for large values of v_{2k}. For this reason, we also consider the potentials

$$V(r) = r^{2k}, \qquad k = 1, 2, 3, 4, \text{ and } 10, \quad (4.5)$$

to cover the limiting case of the anharmonicity constant, as $v_{2k} \to \infty$. The potential in (4.5) with $k = 1$, or (4.1) with $v_{2k} = 0$, corresponds to the harmonic oscillator whose exact eigenstates are given by (1.7) for the unbounded interval of r, $r \in [0, \infty)$. Therefore, this problem provides a very good check on the accuracy of the present approach, which assumes a finite interval, $r \in [0, L]$.

As a specimen test, Table I demonstrates the rate of convergence of the method as functions of

TABLE I
Convergence rate of the method as functions of L and N for the ground-state energy $E_{0,0}$ of the harmonic oscillator, $V(r) = r^2$.

L	N	$E_{0,0}$
5	8	2.000 000 001 346
	10	2.000 000 001 3308
	12	2.000 000 001 33077
7	14	2.000 000 000 000 000 0306
	16	2.000 000 000 000 000 000 1007
	18	2.000 000 000 000 000 000 1006
9	20	2.000 000 000 000 000 000 005 952
	22	2.000 000 000 000 000 000 000 188
	24	2.000 000 000 000 000 000 000 000 00000
11	26	2.000 000 000 000 000 000 0168
	28	2.000 000 000 000 000 000 000 000 0236
	30	2.000 000 000 000 000 000 000 000 00000

the boundary parameter L and the truncation size N in calculating the exact ground-state energy, $E_{0,0} = 2$, of the harmonic oscillator. It is seen that if we restrict ourselves to about 10 digit accuracy, it is sufficient to set $L = 5$. Increasing L from 5 to 7 and to 9, respectively, 20 and 30 significant figures are obtained.

In our numerical tables, we report eigenvalues to 30 digits. Table I shows clearly that this prescribed accuracy is first achieved at $L = 9$, and if we take an L value beyond $L = 9$, for instance, $L = 11$, we certainly get the same result again at the cost of using a higher truncation size. Therefore, $L = 9$ is called the critical or optimum boundary value, denoted by L_{cr}, for this case. Such a behavior of determining eigenvalues with respect to L is observed in all our calculations.

In general, we continue changing L until the eigenvalues of the required accuracy, i.e., 30 digits, are obtained. The definition of L_{cr} implies the statement that

$$|E^{(\infty)} - E(L_{cr})| < \epsilon, \tag{4.6}$$

where $\epsilon = 10^{-30}$ and $E(L)$ and $E^{(\infty)}$ are the eigenvalues of the bounded and the corresponding unbounded problem, respectively. Also, the influence of the finite boundary on the spectrum, numerically speaking, is greater than ϵ when $L < L_{cr}$. Of course, L_{cr} is not a unique value which has to be estimated very precisely. Our computational search shows that in the near vicinity of the reported L_{cr} values the rate of convergence is more or less the same in finding the low-lying state energies. Furthermore, the algorithm employs a minimum number of the basis functions in this neighborhood of L_{cr}. Actually, if $L \gg L_{cr}$, then a considerable slowing down of convergence may occur.

The existence of an optimum value of L, which should not be very small or very large, may also be deduced from the fact that the kinetic energy

TABLE II
Critical values L_{cr} and the energy eigenvalues $\lambda_{n,0}$ of the potential, $V(r) = r^{2k}$, as a function of k.

k	n	$\lambda_{n,0}$	L_{cr}	N
1	0	2.000 000 000 000 000 000 000 000 000 00000	9.0	24
	1	6.000 000 000 000 000 000 000 000 000 00000	9.5	28
	2	10.000 000 000 000 000 000 000 000 000 0000	9.5	30
	3	14.000 000 000 000 000 000 000 000 000 0000	9.5	32
	4	18.000 000 000 000 000 000 000 000 000 0000	10.5	34
2	0	2.344 829 072 744 275 209 808 995 79643	5.0	28
	1	9.529 781 384 014 807 959 799 611 30530	5.0	30
	2	18.735 195 504 701 770 773 554 069 1439	5.0	30
	3	29.301 548 228 942 291 903 145 808 4950	5.0	32
	4	40.941 918 353 803 625 625 662 009 1641	5.25	34
3	0	2.609 388 463 253 714 006 877 033 41876	3.6	34
	1	11.946 863 508 851 368 705 043 604 0993	3.6	36
	2	25.463 626 993 869 977 140 819 711 2200	3.6	36
	3	42.067 859 920 619 309 008 621 746 0328	3.6	38
	4	61.261 386 349 562 942 201 185 703 1423	3.6	38
4	0	2.828 786 159 942 523 348 784 150 37593	2.9	42
	1	13.699 710 847 251 447 928 135 472 2390	2.9	42
	2	30.581 181 755 692 765 465 261 256 2851	2.9	42
	3	52.183 559 593 757 451 059 366 450 9780	2.9	44
	4	77.884 490 773 999 550 572 609 283 8675	2.9	44
10	0	3.651 024 848 669 465 833 849 211 68554	1.72	84
	1	19.019 015 732 785 642 006 588 600 8668	1.72	84
	2	45.936 257 303 451 846 037 295 055 3049	1.72	84
	3	83.598 817 125 768 624 847 870 170 5885	1.72	84
	4	131.346 976 425 067 960 776 224 366 561	1.72	84

term in the variational matrix (2.13) grows unboundedly as $L \to 0$, whereas the potential energy term becomes infinite as $L \to \infty$. On the other hand, the full spectrum of an eigenvalue problem cannot be calculated by estimating a fixed critical distance. Naturally, the larger L_{cr} values are needed for the higher excited states. As a result of these remarks, we may conclude that L_{cr} depends on the required accuracy ϵ, the state number n, and the potential function $V(r)$ in question.

In Tables II and III, we report the first few state energies of the potentials in (4.5) for $l = 0$ and $l = 1$, respectively. It is clear that the number of basis functions N we used increases from 24 to 84 as the potentials vary from harmonic oscillator to the potential $V(r) = r^{20}$. Owing to the contraction of the potentials as k increases, however, L_{cr} decreases.

The eigenvalues of the quartic, sextic and octic anharmonic oscillators are tabulated in Tables IV–VI for a very wide range of the coupling constants. It is worth mentioning that there is no accuracy loss in any regime of the eigenvalues. In these tables, the eigenvalues for $v_{2k} > 1$ are replaced by $v_{2k}^{-1/(k+1)}E$ to show how rapidly they converge to the $v_{2k} \to \infty$ limit energies given in Table II. The rate of convergence in each case is consistent with that of the potential in Table II having the same asymptotic behavior. The numerical data are presented only for $l = 0$ in order not to overfill the content of the article with tabular material anymore. Further results are available from the authors.

Finally, the method is applied to an eigenvalue problem of a different nature, where the potential has two minima in Cartesian coordinates. We see from Table VII that the method has the capability of yielding accurate results in this case as well. In general, the recorded eigenvalues to 30 digits in our tables are in good agreement with the previously published results to the accuracy quoted [5] (and the references therein).

TABLE III
Critical values L_{cr} and the energy eigenvalues $\lambda_{n,1}$ of the potential, $V(r) = r^{2k}$, as a function of k.

k	n	$\lambda_{n,1}$	L_{cr}	N
1	0	4.000 000 000 000 000 000 000 000 000 00000	9	26
	1	8.000 000 000 000 000 000 000 000 000 00000	9.5	28
	2	12.000 000 000 000 000 000 000 000 000 0000	9.5	30
	3	16.000 000 000 000 000 000 000 000 000 0000	9.5	32
	4	20.000 000 000 000 000 000 000 000 000 0000	10.5	34
2	0	5.394 227 164 172 288 035 827 128 08911	5	28
	1	13.811 109 536 873 734 556 089 177 2372	5	30
	2	23.775 788 766 400 460 908 084 504 4638	5	30
	3	34.922 189 824 920 427 180 557 215 2974	5	32
	4	47.042 438 982 602 590 421 409 773 5228	5.25	34
3	0	6.298 495 901 483 604 243 475 867 95748	3.6	34
	1	18.042 624 963 215 149 284 883 606 1618	3.6	36
	2	33.226 111 031 283 994 491 360 615 7976	3.6	36
	3	51.197 907 527 921 898 817 904 695 5520	3.6	38
	4	71.579 036 686 497 045 242 774 490 7208	3.6	38
4	0	6.973 963 604 062 474 495 964 177 5380	2.9	42
	1	21.172 924 759 544 699 545 598 219 3823	2.9	42
	2	40.562 306 275 335 065 280 118 837 1528	2.9	42
	3	64.303 564 967 276 949 092 416 203 5681	2.9	44
	4	91.915 659 881 269 497 907 582 925 9112	2.9	44
10	0	9.234 548 141 850 486 506 709 132 62479	1.72	80
	1	30.496 392 239 950 681 357 948 495 1962	1.72	80
	2	62.906 669 978 234 303 678 956 781 7182	1.72	80
	3	105.705 424 592 282 686 348 235 155 655	1.72	80
	4	158.326 821 543 865 973 806 795 382 263	1.72	82

TABLE IV

Critical values L_{cr} and the energy eigenvalues $E_{n,0}$ of the quartic oscillator, $V(r) = r^2 + v_4 r^4$, as a function of v_4.

v_4[a]	n	$E_{n,0}$	L_{cr}
10^{-3}	0	2.001 995 522 094 708 533 684 913 20578	10.5
	1	6.013 936 098 189 653 073 559 642 74371	
	2	10.037 726 447 540 990 997 168 029 2097	
	3	14.073 268 901 848 599 025 546 920 3647	
	4	18.120 467 854 849 535 519 253 608 5835	
1	0	2.952 050 091 962 874 287 056 570 38705	5.25
	1	10.882 435 576 819 807 243 980 305 2898	
	2	20.661 082 690 597 886 008 613 860 6236	
	3	31.725 128 191 323 846 000 694 493 6603	
	4	43.816 823 442 711 769 292 920 245 9907	
10^3	0	2.351 338 918 312 985 396 323 609 83486	1.6
	1	9.543 744 980 405 963 422 344 031 57957	
	2	18.754 903 714 202 645 896 830 091 2136	
	3	29.326 237 058 380 066 510 244 951 0992	
	4	40.971 122 304 391 642 340 873 918 4630	
10^6	0	2.344 894 220 027 885 068 182 968 20759	0.5
	1	9.529 921 064 696 036 065 423 201 49701	
	2	18.735 392 632 619 681 244 508 244 2998	
	3	29.301 795 163 271 981 703 005 355 0114	
	4	40.94 221 043 942 410 630 883 781 62603	

[a]Eigenvalues for $v_4 > 1$ are $v_4^{-1/3} E_{n,0}$.

TABLE V

Critical values L_{cr} and the energy eigenvalues $E_{n,0}$ of the sextic oscillator, $V(r) = r^2 + v_6 r^6$, as a function of v_6.

v_6[a]	n	$E_{n,0}$	L_{cr}
10^{-4}	0	2.000 598 762 132 326 882 320 348 64889	10
	1	6.007 751 220 149 997 804 295 328 80437	
	2	10.032 542 763 227 701 804 824 865 7460	
	3	14.086 013 194 042 651 079 974 348 5427	
	4	18.178 227 767 416 675 616 115 325 6809	
1	0	3.121 935 474 246 425 991 126 392 39363	3.6
	1	12.914 938 793 084 835 743 473 718 5394	
	2	26.720 687 689 389 101 123 735 627 4174	
	3	43.558 836 621 235 999 594 757 325 0745	
	4	62.954 081 100 886 758 921 519 461 6064	
10^4	0	2.614 732 045 811 295 321 263 037 39260	1.4
	1	11.956 628 506 631 557 144 562 373 9480	
	2	25.476 265 711 477 599 711 336 570 5449	
	3	42.082 827 572 804 005 058 067 242 6942	
	4	61.278 364 418 969 761 486 805 218 6638	

[a]Eigenvalues for $v_6 > 1$ are $v_6^{-1/4} E_{n,0}$.

TABLE VI
Critical values L_{cr} and the energy eigenvalues $E_{n,0}$ of the octic oscillator, $V(r) = r^2 + v_8 r^8$, as a function of v_8.

v_8[a]	n	$E_{n,0}$	L_{cr}
10^{-5}	0	2.000 239 435 330 015 489 836 799 61699	9.2
	1	6.004 995 387 244 901 355 807 670 65716	
	2	10.030 661 401 804 310 454 756 728 4019	
	3	14.106 953 931 490 152 999 688 231 7547	
	4	18.271 189 889 023 522 434 922 736 7644	
1	0	3.287 880 426 306 474 147 366 316 46427	2.9
	1	14.491 330 259 511 367 660 816 113 6330	
	2	31.551 234 380 201 413 588 563 682 1136	
	3	53.294 182 462 089 064 595 699 742 6777	
	4	79.113 049 969 649 292 429 073 078 1720	
10^5	0	2.833 519 160 868 379 169 539 757 15041	0.9
	1	13.707 644 868 712 494 398 947 958 8335	
	2	30.590 894 905 108 705 724 012 094 2824	
	3	52.194 675 854 570 619 011 260 569 8965	
	4	77.896 784 653 678 648 629 907 144 5488	

[a]Eigenvalues for $v_8 > 1$ are $v_8^{-1/5} E_{n,0}$.

In this article, to the best of our knowledge, a Fourier–Bessel expansion for the wave function is utilized for the first time for solving eigenvalue problems of this kind. The accuracy of the method is quite impressive. The evaluation of the matrix elements given in Section 3 requires only the determination of the zeros of Bessel functions accurately. To this end, making use of Mathematica [9], we calculated the zeros to 40 digits.

It is well known, from the variational principle, that the Rayleigh–Ritz method provides an upper bound for the eigenvalues. Therefore, better ap-

TABLE VII
Critical values L_{cr} and the energy eigenvalues $E_{n,0}$ of the two-well potential, $V(r) = -r^2 + d_4 r^4$, as a function of d_4.

d_4	n	$E_{n,0} + 1/(4d_4)$	L_{cr}
10^{-2}	0	1.398 819 606 958 560 193 588 327 78011	15
	1	4.164 445 401 438 967 973 159 747 89411	
	2	6.863 695 271 722 825 702 783 019 62531	
	3	9.491 359 674 405 070 730 025 119 44685	
	4	12.040 996 051 530 290 407 545 701 1565	
1	0	1.637 487 952 723 690 820 759 675 40693	5.25
	1	8.087 207 576 543 170 457 679 953 48886	
	2	16.716 860 324 044 199 941 511 949 9881	
	3	26.785 032 000 948 397 536 055 018 3172	
	4	37.973 893 745 187 635 988 564 044 5983	
10^2	0	10.745 379 344 538 852 199 155 496 0807	2.35
	1	43.934 440 817 669 132 038 133 141 7197	
	2	86.538 410 698 064 907 492 909 114 7669	
	3	135.475 768 778 152 347 645 925 981 316	
	4	189.408 304 514 324 643 004 961 139 847	

proximations are sure to be achieved for successive values of N. On the other hand, it is not surprising that the larger region has smaller eigenvalues for such a boundary value problem. Actually, Nunez [10] showed theoretically that the eigenfunctions of an unbounded system can be approximated by means of the numerical solutions of the Dirichlet problem in the Hilbert space $L_2(\Omega)$ with sufficiently large Ω, where Ω is a bounded region. This makes our strategy plausible in obtaining the eigenvalues of unbounded oscillators by increasing the boundary parameter L. However, our studies on the estimation of error bounds and the generalization of the method to higher-dimensional spaces are in progress and will be reported in the near future.

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